Center for Computational Sciences and Simulation CCSS

UNIVERSITÄT DUISBURG ESSEN

Offen im Denken

Multiferroic composites with strain-induced magneto-electric coupling

FOR 1509 "Ferroic Functional Materials"

The research group focusses on the continuum-mechanical modeling and experimental characterization of ferroic functional materials. The overall aim is to develop a new quality in reliable and robust modeling tools for the description of complex, non-linear, magneto-electro-mechanical interactions on multiple length scales. The coupled two-scale simulation of magneto-electric composites is of particular interest.

`http://www.uni-due.de/ferroics`

Introduction

Materials that exhibit strong magneto-electric (ME) coupling may find application in sensor technology and data storage. Since natural materials generally have low ME coupling at room temperature synthetic (composite) materials consisting of piezoelectric and -magnetic phases become relevant. In such composites ME coupling arises as strain-induced product property [2].

Computational homogenization of ME composites

For the analysis of the coupled behavior of ME composites we take into account the kinematic quantities and balance equations

$$\begin{array}{ccc} \boldsymbol{\varepsilon} = \nabla^s \boldsymbol{u} & \mathbf{E} = -\nabla\phi & \mathbf{H} = -\nabla\varphi \\ \nabla\cdot\boldsymbol{\sigma} + \boldsymbol{f} = \mathbf{0} & \nabla\cdot\mathbf{D} = q & \nabla\cdot\mathbf{B} = 0 \\ \text{(elastostatics)} & \text{(electrostatics)} & \text{(magnetostatics)} \end{array}$$

The effective response of the ME composite is obtained from a representative volume element ($\mathcal{RVE}$). The micro-fields are decomposed into macroscopic part $\overline{\bullet}$ and micro-fluctuations $\widetilde{\bullet}$

$$\boldsymbol{\xi} = \overline{\boldsymbol{\xi}} + \widetilde{\boldsymbol{\xi}} \quad \text{with} \quad \boldsymbol{\xi} := [\boldsymbol{\varepsilon}, \boldsymbol{\sigma}, \boldsymbol{E}, \boldsymbol{D}, \boldsymbol{H}, \boldsymbol{B}] \,.$$

Energetically consistent periodic boundary conditions are computed from a generalized Hill-Mandel condition [3] and are applied along the boundary of the $\mathcal{RVE}$. The homogenized response is computed by averaging over the microscopic fields on the $\mathcal{RVE}$

$$\overline{\boldsymbol{\xi}} := \frac{1}{V_{\mathcal{RVE}}} \int_{\mathcal{B}} \boldsymbol{\xi} \, dv \,.$$

We suppose linear, transversely isotropic material response of the piezoelectric and -magnetic phases on the microscale. The incremental constitutive equations of the individual phases are

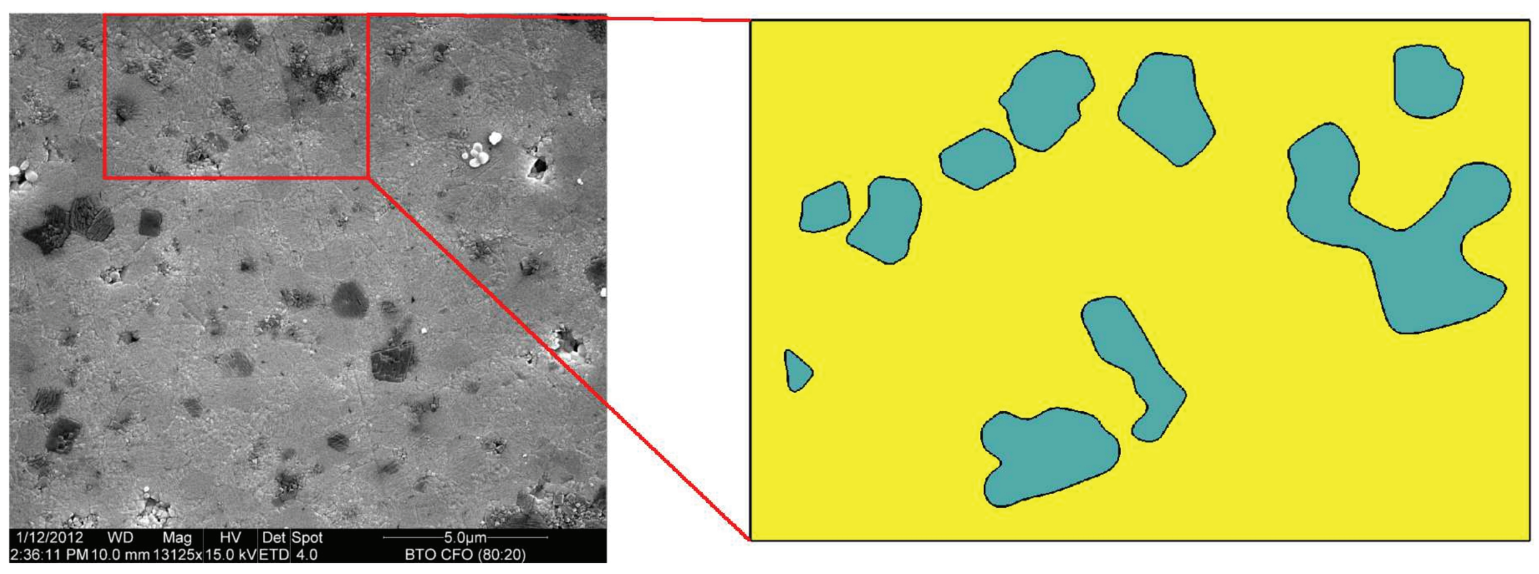
$$\begin{bmatrix} \Delta\boldsymbol{\sigma} \\ -\Delta\boldsymbol{D} \\ -\Delta\boldsymbol{B} \end{bmatrix} = \begin{bmatrix} \mathbb{C} & -\boldsymbol{e}^T & -\boldsymbol{q}^T \\ -\boldsymbol{e} & -\boldsymbol{\epsilon} & -\boldsymbol{\alpha}^T \\ -\boldsymbol{q} & -\boldsymbol{\alpha} & -\boldsymbol{\mu} \end{bmatrix} \begin{bmatrix} \Delta\boldsymbol{\varepsilon} \\ \Delta\boldsymbol{E} \\ \Delta\boldsymbol{H} \end{bmatrix}$$

where the ME coupling modulus of the two phases is zero ($\boldsymbol{\alpha} \equiv \mathbf{0}$). However, the overall macroscopic ME modulus $\overline{\boldsymbol{\alpha}}$ of the composite material is in general non-zero and defined as follows

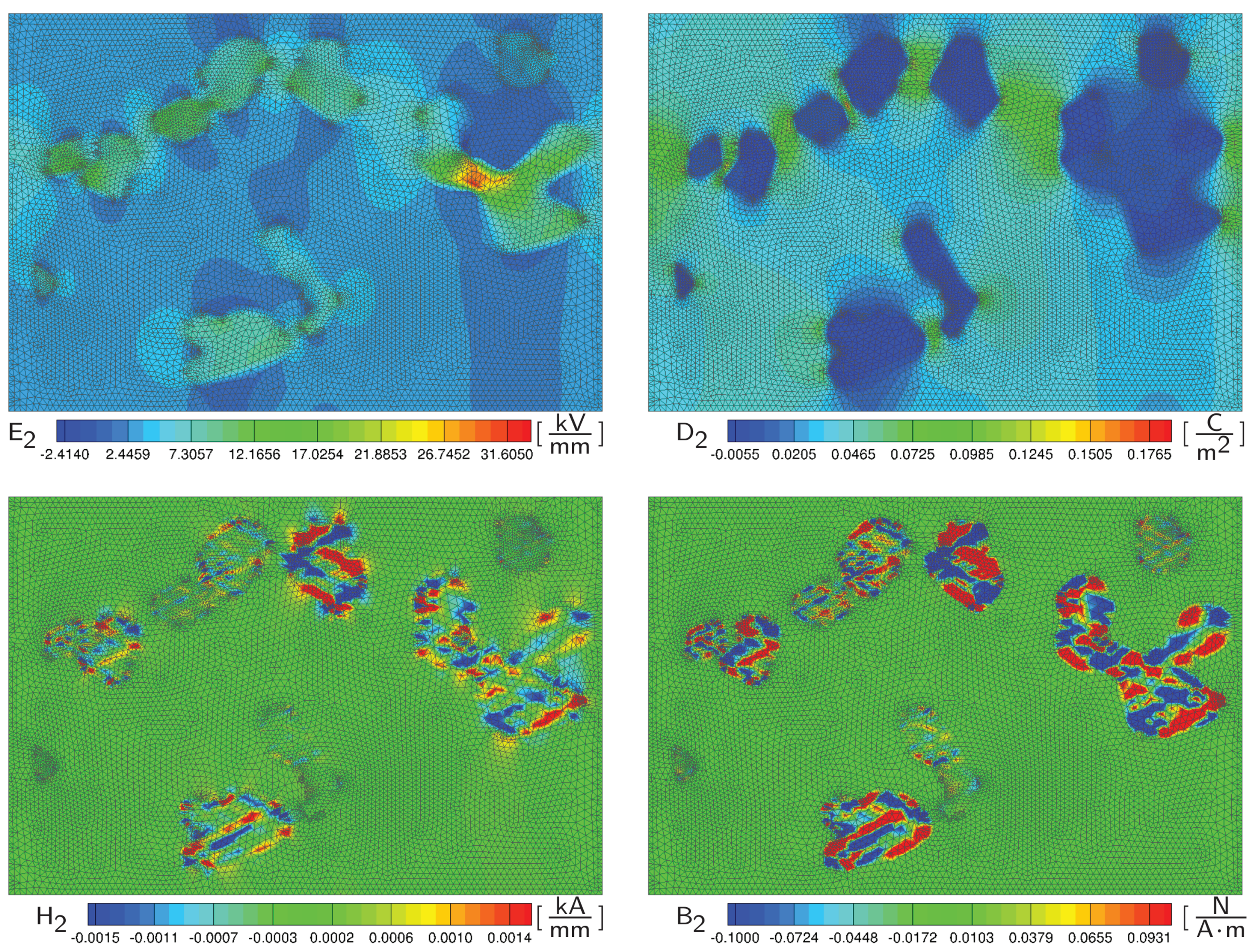
$$\overline{\boldsymbol{\alpha}} = \frac{\partial\overline{\mathbf{B}}}{\partial\overline{\mathbf{E}}} = \left[\frac{\partial\overline{\mathbf{D}}}{\partial\overline{\mathbf{H}}}\right]^T .$$

ME coefficient of experimental micro-structure

We analyze the magneto-electric behavior of a real composite microstructure. The ME composite consists of a piezoelectric matrix ($BaTiO_3$) with embedded particulate piezomagnetic inclusions ($CoFe_2O_4$); the surface fraction of the inclusions is 16%.



In order to analyze the ME coefficient we apply an external electric field $\overline{E}_2$ in vertical direction. The resulting deformation of the piezoelectric matrix is transferred to the piezomagnetic particles so that a (strain-induced) magnetic induction is generated.



The simulated effective ME coefficient $\overline{\alpha}_{22}^{\mathsf{sim}}$ is compared to the experimentally determined coefficient $\overline{\alpha}_{22}^{\mathsf{exp}}$ from [1] ($[\overline{\alpha}] = \frac{N\,s}{V\,C}$)

$$\overline{\alpha}_{22}^{\mathsf{sim}} = 3.893 \cdot 10^{-11} \quad \Leftrightarrow \quad \overline{\alpha}_{22}^{\mathsf{exp}} = 4.4 \cdot 10^{-12} \,.$$

The deviation can be explained by the simplified model assumptions: a) the 2D simulation does not account for the 3D shape of the particulate inclusions, b) the assumed perfect polarity of the individual phases cannot be obtained in experiments. In order to improve the model we will account for highly resolved 3D micro-structures and fundamental non-linearities (polarization and magnetization process). Most efficiently this can be realized by fully coupled FE^2 simulations in a powerfull HPC framework.

References

[1] M. Etier, Y. Gao, V. V. Shvartsman, D. C. Lupascu, J. Landers, and H. Wende, *Proc. Eur. Conf. Applic. Polar Dielec.* 1–4, 2012.

[2] J. Lee, J. G. Boyd and D. C. Lagoudas, *Int. J. Eng. Sci.* 43:790–825, 2005.

[3] J. Schröder and M.-A. Keip, *Comput. Mech.* 50:229–244, 2012.

J. Schröder, M.-A. Keip, M. Labusch
Institute of Mechanics
Department of Civil Engineering
University Duisburg-Essen

D. C. Lupascu
Institute for Materials Science
Department of Civil Engineering
University Duisburg-Essen

DFG
SCHR 570/12–1